# THE FINITE ALGEBRA FOR PERCEPTION OF RINGS IN MOLECULES*

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The communication describes the finite algebra for perception of rings in molecules. It is demonstrated that for an arbitrary spaning tree we may construct the so-called restricted set of rings, which is composed of all possible (dependent and/or independent) rings that are classified by making use of some required constrains as "chemically important". The method makes possible the formulation of efficient algorithms how to exhaustive perceive the rings in molecules.

The perception of rings is an essential part of any computer program for simulation of organic synthesis. It represents the necessary first step in the perception of the chemical nature of the molecular structure, the prediction of its chemical behavior. The presence of rings in a molecular structure is a restriction of chemical reactivity of functional groups within the molecule, reactivity toward common reagents may be substantially altered.

The total number of "independent" rings (this term is fully specified in forthcoming sections) of a connected undirected graph $G$ composed of $N$ vertices and $M$ edges is specified by the so-called cyclomatic number[1] $c(G) = M - N + 1$. A set of $c$ independent rings will be called the fundamental set of rings. We have a large freedom in construction of this set, therefore it is very worthwhile to introduce further restrictions specifying more deeply the set of rings. For instance, one can require that the set of rings is formed of smallest rings. From such a set of rings we can determine the total ring strain energy, aromaticity, topology, and most importantly, the set of synthetically important rings. The ring-perception problems have been studied by many authors[2-12].

The purpose of the present communication is to algebraize the problem of perception of rings by making use of some special kind of finite algebra over the scalar field of modulo 2. This very interesting possibility was initially mentioned by Corey and Peterson[3], now the algebraic approach is used as a powerful formal device to formulate many important concepts and notions in ring-perception problem.

## *Basic Concepts of Graph Representation of Molecules*

A molecular structural formula may be unambiguously expressed[13] as a multigraph with loops (*i.e.* pseudo-multigraph), its vertices are evaluated by atomic symbols.

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Such general representation of molecules is unnecessarily complex for the present purposes, therefore we use another simpler alternative graph-theory way how to determine abstractly the molecular structural formula. Let $G = (V, E)$ be the molecular graph assigned to a molecule, where $V = \{v_1, v_2, \ldots, v_N\}$ is the finite non-empty set of vertices (atoms) and $E = \{e_1, e_2, \ldots, e_M\}$ is the finite set of edges (bonds) which are represented by unordered pairs of vertices from $V$, the bond $e_p = (v_i, v_j)$ is said to be incident with the vertices $v_i$ and $v_j$, diagrammatically this is represented by a continuous line connecting the vertices $v_i$ and $v_j$. In order to get a full correspondence between the concept of molecular graph and the molecular structural formula, the vertices and edges of $G$ should be evaluated by symbols specifying more deeply their chemical nature (type of atoms, multiplicity of bonds, *etc.*). A simple walk of $n$ steps on the molecular graph $G$ is an alternative sequence of $n$ edges and $n + 1$ vertices (for $n \geqq 1$), each vertex (except the first and last) is incident with the preceding and with the succeeding edge, no vertex and no edge occurs (or is visited) more than once. A ring is closed walk where the initial and terminal vertices coincide. The size of ring is equal to the number of its edges. A spanning subgraph of the molecular graph $G$ is a graph obtained from $G$ by deleting a subset of its edges (which may be empty set) but retaining all the vertices of $G$. A tree (containing $n$ edges) is a connected graph which contains no rings, clearly this three has $n + 1$ vertices. A spanning tree $T$ of the molecular graph $G$ is a tree which is the spanning subgraph of $G$, $T = (V, E' \subseteq E)$. A ring-closure edge (determined with respect to the spanning tree $T$) is an edge which was deleted from $E$ in forming the spanning tree $T$ from the graph $G$. The total number of ring-closure edges is determined mined by the so-called cyclomatic number[1]

$$c(G) = M - N + 1\,, \qquad (1)$$

this number is an invariant of the graph $G$ and does not depend on the particular form of the given spanning tree. The total number of independent rings that can be constructed over the graph $G$ is equal to the number of ring-closure edges, *i.e.* to the cyclomatic number (*1*).The number of all possible rings constructed over the graph $G$ may be much more higher than the cyclomatic number (*1*), but among these rings there are such ones that can be expressed as a combination of other rings. Therefore, we introduce a notion of the fundamental set of rings of $c$ independent rings, then all other rings can be expressed as their combinations.

### *Construction of the Fundamental Set of Rings*

The initial step in the construction of fundamental set of rings is the generation of a spanning tree. An arbitrary vertex of the studied molecular graph $G$ may be fixed as the root of the constructred tree. The tree is organized hierarchically[12], going from the top to bottom, the root (the fixed vertex) is placed on 0-level, on the next level (1-level) are placed all the vertices with unit distance from the root, on the next 2-level we place all the vertices with unit distance from vertices placed on the higher 1-level and with the distance equal 2 from the top vertex (root) placed on 0-level, and similarly for the remaining vertices. The vertices placed on the juxtaposed levels are connected by edges belonging to the set $E$, in particular, each vertex from $n$-level is linked merely by *one edge* starting at the higher $(n-1)$-level, see Fig. 1. The vertices with longest distance from the top root are placed on the bottom level, they are linked only with the vertices from the next higher level. The tree is composed of $N$ vertices (by definition), and as a result of its connectivity, it contains $N-1$ edges. The total number of edges in the graph $G$ is $M$, then the number of ring-closure edges (the edges which were not included at the tree) is equal to $M - N + 1$ [*cf.* Eq. (*1*)]. Now, let us have an arbitrary ring-closure edge, applying a back tracing to higher levels in the direction to the root, we start to find other edges of a ring corresponding to the given ring-closure edge. This process is accomplished when it was found that the given two branches of tree are joined together at a common vertex, see diagram *D* in Fig. 1. The similar back-tracing procedure is repeated for all ring-closure edges. Hence, we have constructed the fundamental set of rings, $\{R_1, R_2, ..., R_c\}$, its individual components are subsets of the set $E$, *i.e.* $R_i \subseteq E$ for $i = 1, 2, ..., c$. For illustration, the spanning trees of the graph in Fig. 1 are

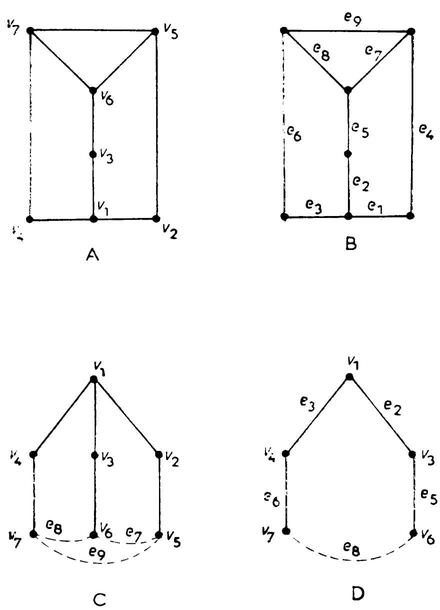


FIG. 1

Illustrative example of the graph $G = (V, E)$. The diagrams A and B present the labeling of $G$ by vertex and edge symbols, respectively. The diagram C is the spanning tree $T(v_1)$ of $G$, the dashed lines are the ring-closure edges. Finally, the diagram D represents the construction of the ring $R_2$ assigned to the ring-closure edge $e_8$

schematically drawn in Fig. 2, the corresponding ring-closure edges and fundamental sets of rings are listed in Table I. Since the rings from a fundamental set are uniquely classified by different ring-closure edges, we may say, formally, that these

TABLE I

Spanning trees

| Root of spanning tree | Ring-closure edges | Fundamental set of rings |
|---|---|---|
| $v_1$ | $e_7, e_8, e_9$ | $\{R_1, R_2, R_3\}$ |
| $v_2$ | $e_5, e_6, e_8$ | $\{R_1, R_3, R_4\}$ |
| $v_3$ | $e_4, e_6, e_9$ | $\{R_1, R_2, R_4\}$ |
| $v_4$ | $e_4, e_5, e_7$ | $\{R_2, R_3, R_4\}$ |
| $v_5$ | $e_2, e_3, e_8$ | $\{R_1, R_3, R_4\}$ |
| $v_6$ | $e_1, e_3, e_9$ | $\{R_1, R_2, R_4\}$ |
| $v_7$ | $e_1, e_2, e_7$ | $\{R_2, R_3, R_4\}$ |

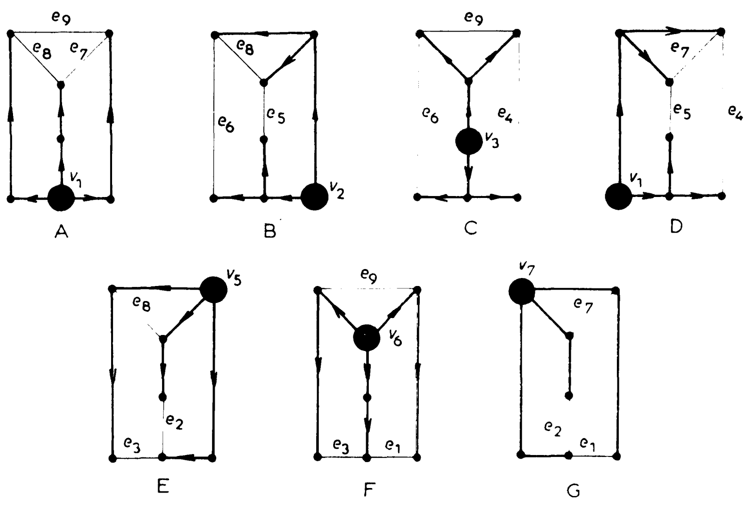


FIG. 2

All possible spanning trees that can be constructed over the graph $G$ determined in Fig. 1, diagrams A and B. The heavy dot denotes the root of spanning tree. The oriented bold-face-lines correspond to the edges included into the given spanning tree, while the thin lines are the ring-closure edges. The orientation of bold-face lines was introduced to facilitate the presentation of hierarchically constructed spanning trees rings are independent. New rings are formed from rings belonging to a fundamental set by making use of the so-called disjoint union[2,3] (or symmetric difference[14], these operations are closely related with the operation "sum" recently used in our communication about the reaction graphs[15]). Let $R$ and $R'$ be two sets, then their disjoint union is determined by

$$R \oplus R' = \{e;\ \text{either } e \in R \text{ or } e \in R',\ \text{but not in both}\}\,. \qquad (2)$$

The rings that can be formed over the graph specified in Fig. 1 are presented in Fig. 3, their "interconversions" according to the binary operation $\oplus$ are listed in Table II. Unfortunately, the disjoint union of rings would produce new "rings" which are not satisfying the ring definition. Let us assume that $R$ and $R'$ are two disjoint rings, $R \cap R' = \emptyset$, then $R \oplus R'$ forms a set of edges which is simple union of $R$ and $R'$, *i.e.* for $R \cap R' = \emptyset$ we get $R \oplus R' = R \cup R'$. This new set $R \oplus R'$ does not correspond to a ring, it contains two rings that may be classified as

1) *fully isolated*, if $R$ and $R'$ have no a common vertex (see first row in Fig. 4), or

2) *spiro*, connected *via* a common vertex, if $R$ and $R'$ share a common vertex (see second row in Fig. 4).

Hence, we have to be very careful in applying the disjoint-union operation over the fundamental set of rings, for a pair of disjoint rings the obtained result $R \oplus R'$ should not a ring.

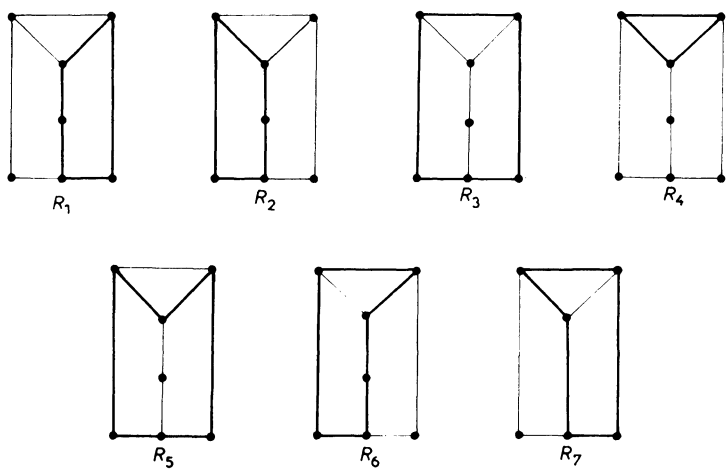


FIG. 3

All possible rings constructed over the graph $G$ determined in Fig. 1, diagrams A and B. The corresponding rings are visualized by bold-face lines

*Finite Algebra of Rings*

Let us have a set of scalars $Z = \{0,1\}$ (integers modulo 2), over the set $Z$ we define an unary operation "$-$" (the complement) and two binary operations "$\oplus$" and "$*$" (the sum and multiplication, respectively), see Table III. The set $Z$ is closed under these operations and forms a field of scalars[16], we say that $Z$ is scalar field modulo 2. Now, let us introduce the cartesian product $Z^M = Z \times Z \times Z \times \ldots \times Z$ of $M$ components, its elements may be formally treated as $M$-tuples (called the vectors) $\boldsymbol{r} = (\alpha_1, \alpha_2, \ldots, \alpha_M)$, where $\alpha_1\ \alpha_2, \ldots \alpha_M \in Z$. This means that the cartesian product $Z^M$ is composed of all possible $M$-tuples, $Z^M = \{(\alpha_1, \alpha_2, \ldots, \alpha_M)\}$, the number of

TABLE II
Multiplication table of rings

| | $\emptyset$ | $R_1$ | $R_2$ | $R_3$ | $R_4$ | $R_5$ | $R_6$ | $R_7$ |
|---|---|---|---|---|---|---|---|---|
| $\emptyset$ | $\emptyset$ | $R_1$ | $R_2$ | $R_3$ | $R_4$ | $R_5$ | $R_6$ | $R_7$ |
| $R_1$ | $R_1$ | $\emptyset$ | $R_5$ | $R_6$ | $R_7$ | $R_2$ | $R_3$ | $R_4$ |
| $R_2$ | $R_2$ | $R_5$ | $\emptyset$ | $R_7$ | $R_6$ | $R_1$ | $R_4$ | $R_3$ |
| $R_3$ | $R_3$ | $R_6$ | $R_7$ | $\emptyset$ | $R_5$ | $R_4$ | $R_1$ | $R_2$ |
| $R_4$ | $R_4$ | $R_7$ | $R_6$ | $R_5$ | $\emptyset$ | $R_3$ | $R_2$ | $R_1$ |
| $R_5$ | $R_5$ | $R_2$ | $R_1$ | $R_4$ | $R_3$ | $\emptyset$ | $R_7$ | $R_6$ |
| $R_6$ | $R_6$ | $R_3$ | $R_4$ | $R_1$ | $R_2$ | $R_7$ | $\emptyset$ | $R_5$ |
| $R_7$ | $R_7$ | $R_4$ | $R_3$ | $R_2$ | $R_1$ | $R_6$ | $R_5$ | $\emptyset$ |

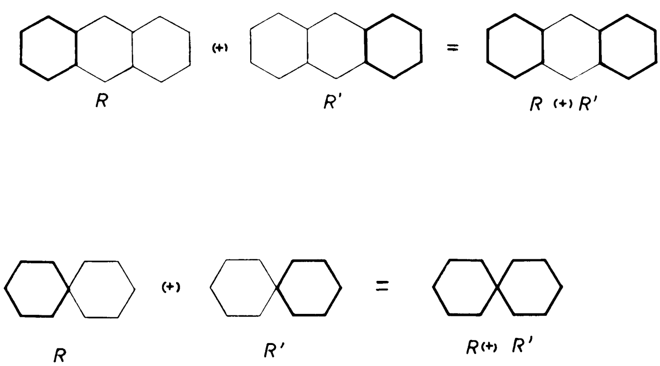


FIG. 4
Two illustrative examples of isolated and spiro rings, respectively, that can be produced when the "sum" operation is applied for a pair of disjoint rings

all its distinct elements is $2^M$. Let us have two vectors $\boldsymbol{r} = (\alpha_1, \alpha_2, \ldots, \alpha_M)$ and $\boldsymbol{s} = (\beta_1, \beta_2, \ldots, \beta_M)$, we define the following three operations over the $Z^M$ and the so-called zero vector.

*1*) the sum of two vectors $\boldsymbol{r}$ and $\boldsymbol{s}$,

$$\boldsymbol{r} \oplus \boldsymbol{s} = (\alpha_1 \oplus \beta_1, \alpha_2 \oplus \beta_2, \ldots, \alpha_M \oplus \beta_M), \quad (3a)$$

*2*) the multiplication of a scalar $\alpha \in Z$ with a vector $\boldsymbol{r}$,

$$\alpha * \boldsymbol{r} = (\alpha * \alpha_1, \alpha * \alpha_2, \ldots, \alpha * \alpha_M), \quad (3b)$$

*3*) the complement to a vector $\boldsymbol{r}$,

$$\bar{\boldsymbol{r}} = (\bar{\alpha}_1, \bar{\alpha}_2, \ldots, \bar{\alpha}_M), \quad (3c)$$

*4*) the zero vector

$$\boldsymbol{0} = (0, 0, \ldots, 0). \quad (3d)$$

The cartesian product $Z^M$ is closed under the operations (*3a – c*) and contains the zero vector $\boldsymbol{0}$. Hence, the cartesian product $Z^M$ can be formally treated as a vector space over the scalar field $Z$. The size $|\boldsymbol{r}|$ of a vector $\boldsymbol{r} = (\alpha_1, \alpha_2, \ldots, \alpha_M)$ is determined as the number of unit elements at its corresponding $M$-tuple. Obviously, the notion of size forms the metric of $Z^M$, *i.e.* $|\boldsymbol{r}| \geqq 0$ for an arbitrary $\boldsymbol{r}$, $|\boldsymbol{r}| = 0$ only for $\boldsymbol{r} = \boldsymbol{0}$, and $|\boldsymbol{r} \oplus \boldsymbol{r}'| \leqq |\boldsymbol{r}| + |\boldsymbol{r}'|$ (the so-called triangular inequivalency).

Now, we turn our attention to the connection[17] of the above introduced finite algebraic theory with our previous considerations about the rings of a molecular graph $G = (V, E)$. Let $R$ be a subset of $E$, $R \subseteq E$, its characteristic function is

$$\chi_R(e) = \begin{cases} 0 & \text{for} \quad e \notin R, \\ 1 & \text{for} \quad e \in R. \end{cases} \quad (4)$$

TABLE III
Algebraic operations

| $\alpha$ | $\beta$ | $\bar{\alpha}$ | $\alpha \oplus \beta$ | $\alpha * \beta$ |
|---|---|---|---|---|
| 0 | 0 | 1 | 0 | 0 |
| 0 | 1 | 1 | 1 | 0 |
| 1 | 0 | 0 | 1 | 0 |
| 1 | 1 | 0 | 0 | 1 |

Then the subset $R$ is unambiguously determined as the following $M$-tuple of zero and unit entries,

$$R \leftrightarrow (\chi_R(e_1), \chi_R(e_2), \ldots, \chi_R(e_M)), \quad (5)$$

an $M$-tuple containing only zero entries corresponds to the empty subset of $E$. For example, the rings listed in Fig. 3 are described by these $M$-tuples

$$\begin{aligned}
R_1 \leftrightarrow \boldsymbol{r}_1 &= (1, 1, 0, 1, 1, 0, 1, 0, 0), \\
R_2 \leftrightarrow \boldsymbol{r}_2 &= (0, 1, 1, 0, 1, 1, 0, 1, 0), \\
R_3 \leftrightarrow \boldsymbol{r}_3 &= (1, 0, 1, 1, 0, 1, 0, 0, 1), \\
R_4 \leftrightarrow \boldsymbol{r}_4 &= (0, 0, 0, 0, 0, 0, 1, 1, 1), \\
R_5 \leftrightarrow \boldsymbol{r}_5 &= (1, 0, 1, 1, 0, 1, 1, 1, 0), \\
R_6 \leftrightarrow \boldsymbol{r}_6 &= (0, 1, 1, 0, 1, 1, 1, 0, 1), \\
R_7 \leftrightarrow \boldsymbol{r}_7 &= (1, 1, 0, 1, 1, 0, 0, 1, 1).
\end{aligned}$$

The disjoint union of two rings $R$ and $R'$ (their vector representation is $\boldsymbol{r}$ and $\boldsymbol{r}'$) is realized as follows

$$R \oplus R' \leftrightarrow \boldsymbol{r} \oplus \boldsymbol{r}'. \quad (6)$$

This can be simply verified for the above rings $R_1$ to $R_7$, using the production Table II, we get

$$R_1 \oplus R_2 = R_5 \leftrightarrow \boldsymbol{r}_5 = \boldsymbol{r}_1 \oplus \boldsymbol{r}_2,$$

$$R_1 \oplus R_3 = R_6 \leftrightarrow \boldsymbol{r}_6 = \boldsymbol{r}_1 \oplus \boldsymbol{r}_3,$$

*etc.*

A set of vectors $\{\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_c\}$ is linearly independent if the relation

$$\alpha_1 * \boldsymbol{r}_1 \oplus \alpha_2 * \boldsymbol{r}_2 \oplus \ldots \oplus \alpha_c * \boldsymbol{r}_c = \boldsymbol{0}$$

is satisfied only for zero coefficients $\alpha_1, \alpha_2, \ldots, \alpha_c \in Z$, in the opposite case the vectors are linearly dependent. In the previous section we have vaguely stated that the rings of fundamental set are independent, now we have available the algebraic device how to fill this notion. Let $\mathbf{R} = \{R_1, R_2, \ldots, R_c\}$ be the fundamental set of rings, its algebraic counterpart is a set of associated $c$ vectors $\{\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_c\}$. We say that the rings of $\mathbf{R}$ are independent only if the vectors $\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_c$ are linearly independent, in the opposite case the rings are not independent. By using these relatively simple algebraic tools we shall prove that the rings forming the fundamental set are independent. Let us assume that we have constructed for the graph $G = (V, E)$ a spanning tree $T(v)$, where $v \in V$ is the root. The corresponding ring-closure edges are indexed by $e_1, e_2, \ldots, e_c$, a ring assigned to an edge $e_i$ is then denoted by $R_i$ (for $i = 1, 2, \ldots, c$)

Then the associated vectors $\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_c$ have the following form

$$\begin{aligned} \boldsymbol{r}_1 &= (1, 0, \ldots, 0, x, \ldots, x)\,, \\ \boldsymbol{r}_2 &= (0, 1, \ldots, 1, x, \ldots, x)\,, \\ &\vdots \\ \boldsymbol{r}_c &= 0, 0, \ldots, 1, x, \ldots, x)\,, \end{aligned}$$

where the last $M - c$ entries are symbolically expressed by $x = 0, 1$. Obviously, these vectors are linearly independent, which immediately implies that the elements of an arbitrary fundamental set of rings, constructed with respect to an arbitrary spanning tree $T(v)$, are independent.

For our forthcoming considerations it will be of great importance to know how many distinct (linearly dependent and independent) vectors can be constructed by linear combinations of the vectors $\{\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_c\}$ [the algebraic counterpart of the fundamental set of rings constructed with respect to a spanning tree $T(v)$]. Since in the framework of the present finite algebra the following lemma is satisfied: $\boldsymbol{r} \oplus \boldsymbol{r}' \neq \boldsymbol{r} \oplus \boldsymbol{r}''$ implies $\boldsymbol{r}' \neq \boldsymbol{r}''$, a pair of different linear combinations of vectors produces the different vectors. Generalizing this property, a linear combination $\alpha_1 * \boldsymbol{r}_1 \oplus \ldots \oplus \alpha_c * \boldsymbol{r}_c = \boldsymbol{r}$ determines uniquely the resulting vector $\boldsymbol{r}$. Hence, we may simply enumerate all distinct vectors that are induced by the set $\{\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots$ $\ldots, \boldsymbol{r}_c\}$, we get

$$\binom{c}{0} + \binom{c}{1} + \binom{c}{2} + \ldots + \binom{c}{c} = 2^c\,, \qquad (8)$$

where $\binom{n}{m}$ is the binomial coefficient $n!/m!(n - m)!$, the term $\binom{c}{i}$ is the number of all different combinations of $i$ vectors from the set $\{\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_c\}$, and $\binom{c}{0}$ corresponds to the zero vector $\boldsymbol{0}$. Summarizing, for a preselected spanning tree $T(v)$ with $c$ ring-closure edges, the corresponding set of vectors is composed of $c$ linearly independent vectors, and moreover, this set induces a $c$-dimensional space $U_{T(v)} \subseteq \mathbf{Z}^M$ which contains $2^c$ different vectors.

Let us consider two spaces $U_{T(v)}$ and $U_{T(v')}$ that are constructed with respect to different spanning trees $T(v)$ and $T(v')$, respectively, where $v \neq v'$ and $v, v' \in V$. We have proved that both these spaces are $c$-dimensional and are composed of $2^c$ different vectors. The spaces $U_{T(v)}$ and $U_{T(v')}$ are induced by the sets of linearly independent vectors $\{\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_c\}$ and $\{\boldsymbol{r}'_1, \boldsymbol{r}'_2, \ldots, \boldsymbol{r}'_c\}$ assigned to the fundamental sets of rings $\mathbf{R} = \{R_1, R_2, \ldots, R_c\}$ and $\mathbf{R}' = \{R'_1, R'_2, \ldots, R'_c\}$, respectively. In accordance with the determination of spanning tree, any ring that can be constructed over the molecular graph $G$ should be ($i$) immediately contained at a fundamental set of rings related to an arbitrary spanning tree, or ($ii$) expressed as a combination (disjoint-union operation) of rings belonging to the fundamental set. Consequently, an arbitrary vector $r'_i \in \{r'_1, r'_2, ..., r'_c\}$ is unambiguously determined as the linear combination of vectors from $\{r_1, r_2, ..., r_c\}$,

$$r'_i = \alpha_1 * r_1 \oplus \alpha_2 * r_2 \oplus ... \oplus \alpha_c * r_c . \qquad (9)$$

Hence, the spaces $U_{T(v)}$ and $U_{T(v')}$ induced by different sets of vectors $\{r_1, r_2, ..., r_c\}$ and $\{r'_1, r'_2, ..., r'_c\}$, respectively, are identical

$$U_{T(v)} \equiv U_{T(v')} , \qquad (10)$$

for any pair of spanning trees $T(v)$ and $T(v')$ related to different roots $v \neq v'$. This principal property is of the great importance for our forthcoming considerations, it states that any possible spanning tree may be preselected as a starting point for the construction of the space $U$, all spanning trees give the same space $U$.

*Construction of a Set of Rings Satisfying Prescribed Restrictions*

Let us assume that we have constructed a fundamental set of rings $\mathbf{R} = \{R_1, R_2, ... ..., R_c\}$ relative to a spanning tree $T(v)$. Now, we would like to construct from this fixed fundamental set $\mathbf{R}$ a new set of rings that are satisfying some class of restricting conditions. Usually, these conditions are formulated in such a way that the resulting rings belong to a family of chemically important rings from the standpoint of solved problem. For example, a constructed set of rings is determined by requiring that their size is less than a threshold.

Following the previous section, an arbitrary vector $r \in U$ is uniquely determined by the linear combination of vectors from the basis set $\{r_1, r_2, ..., r_c\}$,

$$r = \beta_1 * r_1 \oplus \beta_2 * r_2 \oplus ... \oplus \beta_c * r_c , \qquad (11)$$

where $\beta_1, \beta_2, ..., \beta_c \in Z$. The right-hand side of (*11*) may be formally expressed as the following $c$-tuple

$$r = [\beta_1, \beta_2, ..., \beta_c] . \qquad (12)$$

Hence the space $U$ is composed of $c$-tuples (*12*), but now these $c$-tuples must be related to the fixed set of vectors $\{r_1, r_2, ..., r_c\}$. The set of restricted vectors, $U_{restr}$, is formally determined as follows

$$U_{restr} = \{r; r \in U \text{ and } P(r)\} \subseteq U . \qquad (13)$$

It means that the set $U_{restr}$ is composed of those vectors $r \in U$ for which the statement $P(r)$ (restricting conditions and a check whether the vector $r$ correspond to the notion of ring or not) is true. The restricted set of rings, $\mathbf{R}_{restr}$, is then immediately constructed from the rings assigned to the vectors $\boldsymbol{r} \in U_{restr}$,

$$\mathbf{R}_{restr} = \{R;\ R \leftrightarrow \boldsymbol{r} \text{ and } \boldsymbol{r} \in U_{restr}\}\,, \qquad (14)$$

its cardinality (number of elements) may be, in general, different of the cardinality of fundamental set of rings, *i.e.* $|\mathbf{R}_{restr}| \neq |\mathbf{R}| = c$. If $|\mathbf{R}_{restr}| = |\mathbf{R}| = c$ and the set $\mathbf{R}_{restr}$ is composed of independent rings, then $\mathbf{R}_{restr}$ is called the restricted fundamental set of rings.

## SUMMARY

The algebraic theory outlined at the previous sections belongs among standard topics of algebraically oriented graph-theory textbooks[17]. We believe that its consequent application to the problem of perception of rings in molecule offers very effective possibilities how to exhaustive preceive and enumerate all the possible rings that are satisfying some class of restricting conditions. To the knowledge of authors, such a possibility has not been consequently used. Usually, the problem of construction of a restricted set of rings is solved by making use of a preselected spanning tree with an additional application of more or less ingenious heuristics, which may potentially, considerably accelerate the process of finding the rings that are satisfying prescribed restricting conditions. But what is slightly discouraging there, almost each author of such a procudere usually presents a few counter examples unproperly determined by his suggested method.

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